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14. ABSTRACT
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Model reduction is a promising technique to substantially reduce the computational cost involved in the propagation of uncertainty. This collaborative project has provided new algorithmic tools and analyses for model reduction of nonlinear systems, demonstrated their application to various systems including uncertainty quantification in chemically reacting flows, and developed adaptive stochastic collocation methods for optimization problems governed by partial differential equations with uncertain inputs.

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COLLABORATIVE RESEARCH: MODEL REDUCTION FOR PROBABILISTIC ANALYSIS
AND DESIGN UNDER UNCERTAINTY

FA9550-09-1-0225, FA9550-09-1-0239

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Abstract

Effective computational tools to support decision-making under uncertainty are becoming essential in the design and operation of aerospace systems. The accurate and efficient propagation of uncertainties in parameters through complex, high fidelity computational models is a significant challenge. Since analytical characterizations of uncertainties in the system outputs are typically not available, numerical methods must be used that require repeated evaluations of models at suitably sampled parameters.

Model reduction is a promising technique to substantially reduce the computational cost involved in the propagation of uncertainty. This collaborative project has provided new algorithmic tools and analyses for model reduction of nonlinear systems, demonstrated their application to various systems including uncertainty quantification in chemically reacting flows, and developed adaptive stochastic collocation methods for optimization problems governed by partial differential equations with uncertain inputs.

1   Introduction

Effective computational tools to support decision-making under uncertainty are becoming essential in the design and operation of aerospace systems. The accurate and efficient propagation of uncertainties in parameters through complex, high fidelity computational models is a significant challenge. Since analytical characterizations of uncertainties in the system outputs are typically not available, numerical methods must be used that require repeated evaluations of models at suitably sampled parameters. This project develops, analyses, and applies reduced-order models (ROMs) to replace high-fidelity simulations in decision-making under uncertainty. By systematic extraction of key dynamics, model reduction provides an accurate, computationally inexpensive, low-order approximation of the input-to-output map of the system.

We construct projection based ROMs using Proper Orthogonal Decomposition (POD) with snap-

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shots generated using a goal oriented approach. To allow the fast and accurate evaluation of ROMs for a class of parametrically varying systems we have expanded the discrete empirical interpolation method (DEIM) and we have provided state space error estimates for the DEIM.

We have successfully applied our approaches to a number of model problems with relevance to the Air Force. In collaboration with AFRL we have implemented our methods in their codes for fluid-structure interaction applications. Additionally, we have generated ROMs for a challenging reacting flow PDE system. Our approach delivers computational speedups of several magnitudes, while still maintaining accurate predictions of reaction dynamics. This reduction of the forward problem is essential if the effects of uncertainties are to be accounted for, a critical challenge for controlling and reducing emissions.

Finally, we have analyzed the numerical solution of stochastic PDE constrained optimization problems using stochastic collocation. Our method is based on adaptive sparse grid stochastic collocation that adapts the sample size based on the progress of the optimization, thereby reducing the overall computation effort while still guaranteeing convergence.

2 Accomplishments

Many engineering systems can be abstratcly written as

$$\dot{y}(t) = f(y(t), u, \theta, t) \qquad\qquad t \in (0, T), \qquad\qquad \text{(1a)}$$
$$z(t) = g(y(t), u, t) \qquad\qquad t \in (0, T), \qquad\qquad \text{(1b)}$$

where $y(t) \in \mathbb{R}^N$ is the system state ($y(t)$ are, for example, velocities and pressure at time t), u are the possibly time dependent inputs (design variables, controls), θ are possibly uncertain system parameters), and $z(t) \in \mathbb{R}^k$ are the outputs of interest. In optimal control or optimal design, for example, one wants to minimize the integral of z over some set of admissible controls/designs u subject to the state equation (1a). In uncertainty quantification, one wants to determine the statistical properties of the output of interest z given uncertain system parameters θ. Both tasks require the evaluation of many state equations (1a) and, in the optimization context, associated adjoint equations for varying inputs u or θ. For complex systems this becomes prohibitively expensive. Model reduction is a promising technique to substantially reduce the computational cost involved in the propagation of uncertainty or optimization.

Our research studies projection based reduced order models of the form

$$\dot{\hat{y}}(t) = \mathcal{W}^T f(\mathcal{V}\hat{y}(t), u, \theta, t) \qquad\qquad t \in (0, T), \qquad\qquad \text{(2a)}$$
$$\hat{z}(t) = g(\mathcal{V}\hat{y}(t)(t), u, \theta, t) \qquad\qquad t \in (0, T), \qquad\qquad \text{(2b)}$$

where $\hat{y}(t) \in \mathbb{R}^n$ is the reduced system state, $n \ll N$. As before, u are the inputs and $\hat{z}(t) \in \mathbb{R}^k$ are the outputs of interest, which are now generated via a reduced state equation (2a). The matrices

$\mathcal{V}, \mathcal{W} \in \mathbb{R}^{N \times n}$ satisfy $\mathcal{W}^T \mathcal{V} = I$. We have have successfully applied our model reduction approach to examples ranging from uncertainty quantification in chemically reacting flows §2.1, §2.3.1, fluid structure interaction §2.3.2, simulation of nonlinear miscible viscous fingering in a 2-D porous medium §2.3.3, and shape optimization of microfluidic biochips §2.4.

One algorithmic challenge in designing reduced order models is the evaluation of the reduced order model at a computational cost proportional to the size n of the reduced order model. Naive evaluation of (2a), for example, required the evaluation of $\mathcal{V}\widehat{y}(t) \in \mathbb{R}^N$, evaluation of the high fidelity residual $f(\mathcal{V}\widehat{y}(t), u, \theta, t)$, and then projection into a low dimensional subspace via $\mathcal{W}^T$, which is as expensive as evaluating the high fidelity model (1a). The have developed the discrete empirical interpolation method (DEIM), which approximates $\mathcal{W}^T f(\mathcal{V}\widehat{y}(t), u, \theta, t)$ by a function $\widehat{f}(\widehat{y}(t), u, \theta, t)$ that can be evaluated at a cost proportional to $n \ (\ll N)$. The error of the additional approximation due to the DEIM can be controlled and we have provided state-space error estimates for the DEIM reduced order models. See §2.3.4.

Another focus of our research is the numerical solution of optimization problems governed by partial differential equations with uncertain parameters. Here one wants to find optimal controls or optimal designs u that minimize the expected value (or a risk measure) of the output z over all possible parameters θ. The numerical solution of these problems requires iterative methods that for current approximation of the optimal control/design u require the repeated evaluation of (1a) at samples of the uncertain parameters θ. We have developed and analyzed a method based on adaptive sparse grid stochastic collocation that adapts the sample size based on the progress of the optimization, thereby reducing the overall computation effort while still guaranteeing convergence. See §2.2.

Our research has resulted in the publications [1, 2, 3, 4, 5, 7, 9, 8, 10, 11, 13, 14] and theses [6, 12].

2.1 Model Reduction and Uncertainty Quantification in Chemically Reacting Flows

Simulation of reacting flows requires the numerical integration of a system of nonlinear PDEs coupling conservation of mass, momentum and energy; equations of state; and equations describing the chemical source terms. Solving these systems is particularly challenging due to the stiffness of the embedded kinetics and the high computational cost of integrating the nonlinear source term that arises from the chemical models. To address these challenges a POD-based approach to obtain efficient ROMs of chemically reacting flows is proposed [4]. The method combines the classical Galerkin projection technique with the efficient interpolation procedure of the DEIM achieving substantial reduction in the total number of degrees of freedom, providing a systematic means to derive models that are fast to solve but retain high-fidelity predictive capability.

The method was applied to a simplified model of a premixed H_2-Air flame at constant and uniform pressure. The evolution of the flame is governed by a nonlinear system of two-dimensional
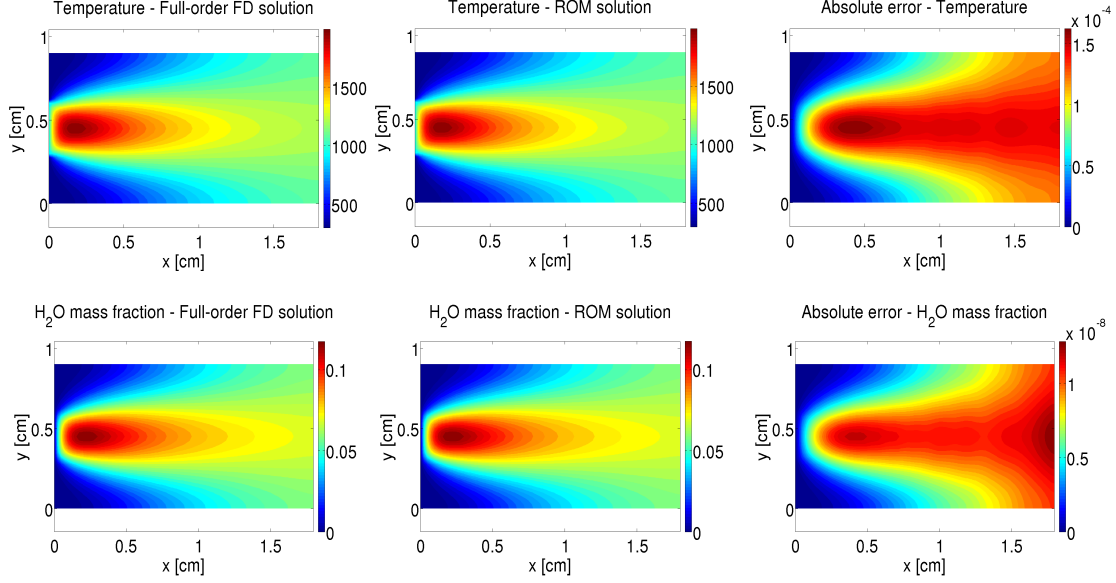
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Figure 1: Comparison of full-order model and reduced-order model simulations at steady-state. The reduced-order model is constructed using 40 POD modes and 40 DEIM interpolation points

convection-diffusion-reaction PDEs, with nonlinear reaction source term of Arrhenius type and chemistry modeled by an irreversible one-step reaction: $2H_2 + O_2 \rightarrow 2H_2O$. The nonlinear system of PDEs was discretized using the finite difference method (FD) and has $N = 10804$ states. Figure 1 shows a comparison of the full and reduced solutions obtained at steady-state and the corresponding absolute error distribution over the computational domain for temperature and H_2O mass fraction. The figure shows that the reconstructed solutions are almost identical to their full-order FD counterparts. The CPU time required by the reduced-order model to reach the steady-state solution is 1000 times smaller than that required by the full-order simulation.
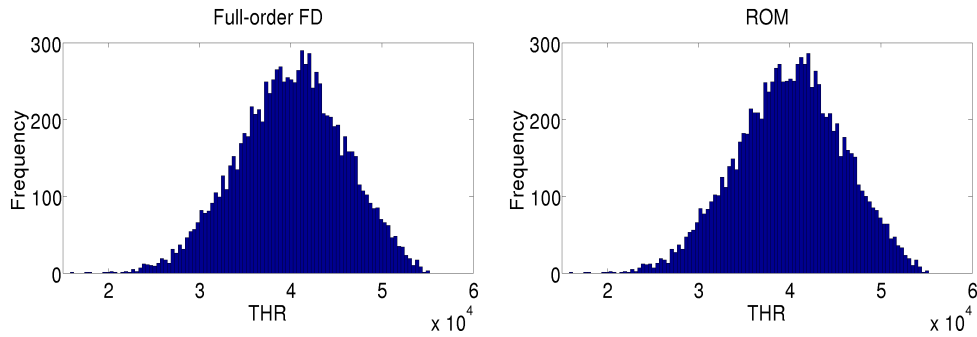

Figure 2: Comparison of full-order FD model and ROM predictions of total heat release (THR). Monte Carlo simulation results are shown for 10,000 different Arrhenius parameters.

Figure 2 shows the results of a Monte Carlo (MC) simulation to analyze the impact in the total

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heat release (THR) of changes in the Arrhenius parameters, e.g. the pre-exponential rate constant and the activation energy, that control the chemical reaction rate. The THR is a measure of the total power released by the combustion and it is defined as the integral over the domain of the heat release due to combustion. The case presented in Figure 2 considers the solution of the

	Full-order FD	Reduced-order model
Model dimension	10804	40
Offline cost (seconds)	–	1.2153e+03
Online cost (seconds)	1.1758e+05	6.3589e+01
THR mean	3.9973e+04	3.9981e+04
THR variance	3.3598e+07	3.3644e+07

Table 1: Full-order model and ROM MCS results. Total heat release is predicted for 10000 different Arrhenius parameters.

steady version of the nonlinear system of PDEs governing the flame. To model the uncertainty in the Arrhenius parameters, $K = 10000$ parameter values were sampled randomly from log-normal distributions, the first having mean 5.5e+12 and variance 9.5e+24, and the second having mean 5.5e+03 and variance 3.0e+06. The corresponding solutions were computed using both the full-order FD model and a ROM of dimension 40. Figure 2 shows the resulting probability density functions for the total heat release. The results for the MC simulations are summarized in Table 1. The ROM is able to predict the mean, variance and shape of the distribution of THR accurately, slashing the computational time required by the MC simulation by a factor of 1800.

2.2 Stochastic Collocation Methods for the Solution of Optimal Control Problems Governed by PDEs with Stochastic Inputs

Many optimal control or design optimization problems involve uncertain inputs (e.g., in the form of material parameters or geometries). In these cases the governing PDEs become a family of equations indexed by a stochastic variable and the solution of the PDE with uncertain inputs are random fields. We have provided an infinite dimensional framework based in Bochner spaces for such optimization problems, and we have established existence results and optimality conditions for classes of problems. We have extended the stochastic collocation method to the optimization context and explored the decoupling nature of this method for gradient and Hessian computations. Furthermore, we have provided a-priori estimates for the error between the solution of the infinite dimensional optimization problem and its stochastic collocation - finite element discretization.

Figures 3 and 4 show computational results for an optimal control problem. The control is the temperature of a fluid at the inflow boundary $\{0\} \times (0, 0.75)$ and the objective is to obtain a temperature in the solid region $(0.75, 1) \times (0, 1)$ that is close to 90 C. Diffusivities in the solid and fluid subdomains and the heat source are random variables. Figure 4(a) shows that it is not enough to
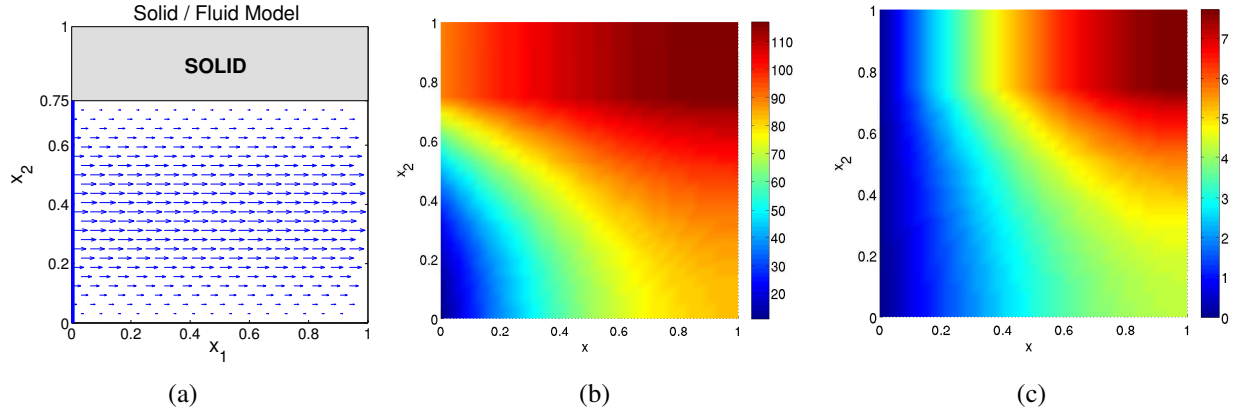
Figure 3: The domain with control boundary plotted in blue is shown in (a). Plots (b) and (c) show the expected value and standard deviation of the optimal state. Both were computed using piecewise linear finite elements on a uniform mesh ($h = 1/32$) and sparse grid collocation with $Q = 129$ points.
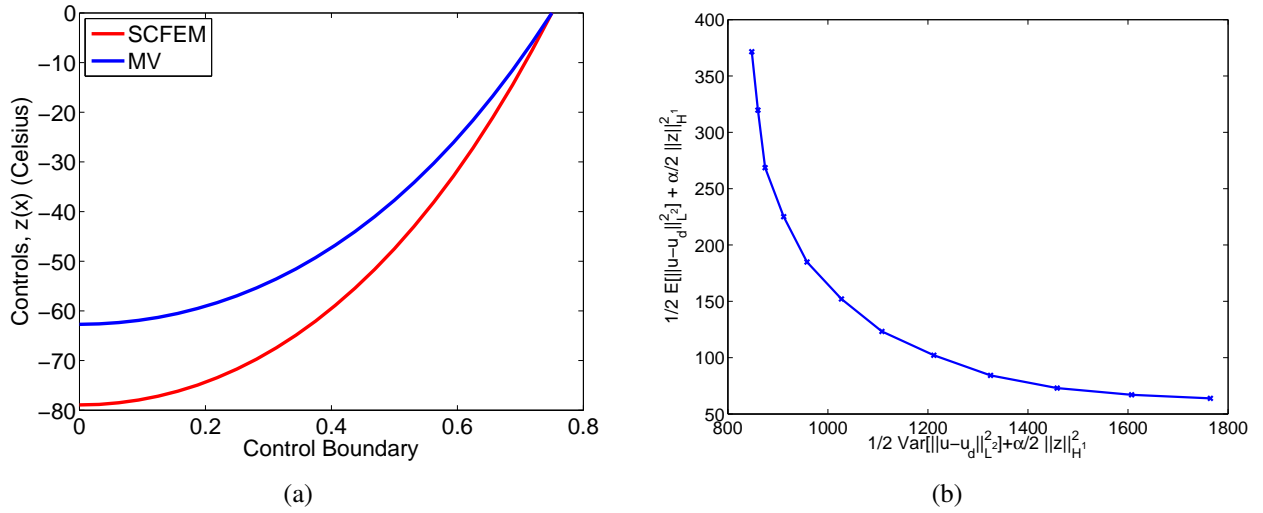

Figure 4: Plot (a) show the optimal controls computed by solving the stochastic optimization problem (red curve) and a deterministic optimization problem in which the random inputs are replaced their mean values (blue curve). The two solutions differ by up to 30%, which underlines the importance of properly including stochastic inputs through stochastic optimization. Plot (b) shows the Pareto curve, which represents optimal values when the objective is a convex combination of expected value and variance, and which is important for trade-off studies.

simply replace the uncertain inputs by their mean values and solve the resulting deterministic problem. Instead, solving the stochastic optimization problem provides information about the statistics of the state (such as expected value and standard deviation shown in plots (b) and (c) in Figure 3). It also allows trade-of studies illustrated by the Pareto curve in Figure 4(b), which shows how

much 'risk', measured by variance needs to be assumed to reduce the expected value. The variance can be replaced by coherent risk measures is ongoing.

2.3   The Discrete Empirical Interpolation Method (DEIM)

The DEIM and basic error estimates are described in the papers [7, 9, 8] and the thesis [6].

DEIM computes an approximation $\widehat{f}(\widehat{y}(t), u, \theta, t)$ of $\mathcal{W}^T f(\mathcal{V}\widehat{y}(t), u, \theta, t)$ using a sampling of the nonlinearity and interpolation. Initially, DEIM was developed for problems in which the $i$the component of $f(y, u, \theta, t)$ depends only on the ith component (or a few components) of the unknown y. This is the case in finite difference or finite element discretizations of PDEs. Additionally, we have extended the application of DEIM to problems where $f(y, u, \theta) = \sum_{j=1}^{M} A_j(\theta)y + Bu$ and M is large. This problem structure arises in shape optimization problems such as those in [1], but also in several problems where coefficient functions in PDEs depend on uncertain coefficients. The reduced order model is of the form $\mathcal{V}^T F(\mathcal{V}\widehat{y}, p, u) = \sum_{j=1}^{M} \mathcal{V}^T A_j(p)\mathcal{V}\widehat{y} + Bu$ and is expensive to evaluate for varying p if M is large. DEIM generates a reduced order model of the type $\widetilde{F}(\widehat{y}, u, \theta) = \sum_{j=1}^{m} \widetilde{A}_j(\theta)\widehat{y} + Bu$ with $m \ll M$, which can be evaluated eficiently. In shape optimization problems, where θ represents the vector of shape parameters, this has the additional advantage that one does not need to compute derivatives of a large number of matrices $A_j(\theta)$, $j = 1, \ldots, M$, but only for a few matrices $\widetilde{A}_j(\theta)$, $j = 1, \ldots, m \ll M$.

2.3.1   DEIM Application to Reacting Flow

We have presented computational results already in §2.1. The results in §2.1 focus on the approximation quality of the computed reduced order model. In this section, we report on the computational efficiency.

The numerical simulation of chemically reacting flows leads to a system of the type (1) where y represents the flow variables and the concentrations of the species. The dynamics f are highly nonlinear. Proper orthogonal decomposition (POD) based reduced order models lead to (2). Because of the nonlinearityies in f these models cannot be evaluated efficiently.

Figure 5 shows the performance of POD on this problem in terms of accuracy (measured by relative error of the state reconstruction) and simulation time. The POD reduced order model is able to faithfully reproduce the high fidelity model, but the computational savings are marginal. Figure 5 also shows that using POD-DEIM reduced order model can be computed that achieve excellent accuracy (close to that of POD), provided that a sufficiently large number of DEIM interpolation points are used, and at the same time provide significant computational speedup The efficiency of the POD-DEIM model, allows us to consider the effects of uncertainties (e.g., in boundary conditions, initial conditions, or reaction rates) on the performance of the reacting flow system.
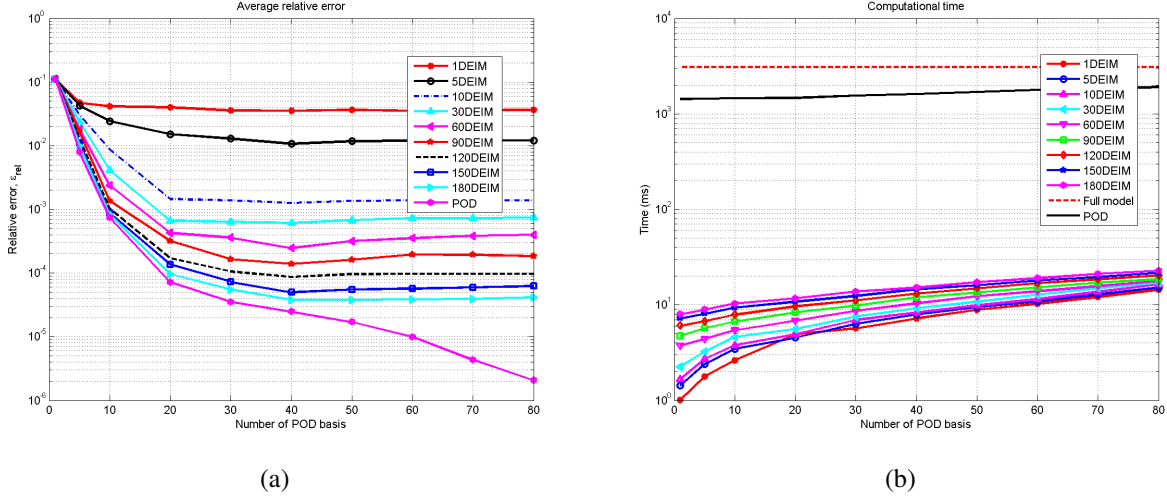
Some of these results were reported in §2.1.

Figure 5: Gaussian laminar flame: a) Comparison of the relative error of the POD, POD-DEIM method. b) Comparison of the computational time of the full model, POD and POD-DEIM method.

2.3.2 DEIM Application to Fluid-Structure Interaction.

As a fluid-structure interaction test case, we are considering the aeroelastic behavior of a cantilevered plate submersed in a supersonic flow. In particular, we consider the example from Stanford and Beran (2010), which aims to minimize structural mass of the plate subject to a constraint on the amplitude of limit cycle oscillation (LCO). This test case will demonstrate the application of our POD-DEIM methods to a new class of problems. It will also demonstrate how our methods can be easily implemented in existing Air Force simulation codes.

For numerical solution, the flat plate is discretized into discrete Kirchhoff theory (DKT) and linear strain triangle (LST) triangular elements. The supersonic flow is modeled by quasi-steady piston theory. The governing equation of motion has a nonlinear internal force term P, which is a function of the displacement vector u due to von Karman strains. This nonlinear force couples in-plane and out-of-plane degrees of freedom. We are currently working with a code provided by AFRL, which simulates the unsteady LCO response of the plate by solving the governing equation in full order. Our goal is to apply POD-DEIM to achieve speed-up in the unsteady solution while introducing minimal changes to the existing code. One challenge is that the nonlinear term $P(u)$ is computed and assembled on an element-by-element basis. Therefore, it cannot be simply evaluated componentwise at the solution vector (as needed for DEIM). Instead, each component of P depends on multiple components of u. This issue can be resolved by passing a matrix containing connectivity information at each node (i.e., the subset of components of u necessary to evaluate each component of P), into the function evaluating the nonlinear force term. This slight modification should allow the application of DEIM to the nonlinear term for this problem. We plan to compare our

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POD-DEIM results to recent results published by AFRL that employ only POD. We will also introduce uncertainties in structural parameters and explore the sensitivity of the LCO response to these uncertainties.

2.3.3 DEIM Application to Simulation of Nonlinear Miscible Viscous Fingering in a 2-D Porous Medium

We have applied DEIM to construct a reduced-order model of a finite difference discretized system used to simulate nonlinear miscible viscous fingering in a 2-D porous medium. The model and additional results are documented in [8].

Figure 6 and Table 2 show results from the application of DEIM. Table 2 show the computational cost of solving the high fidelity finite difference model (which corresponds to (1a) in the abstract setting). If a proper orthogonal decomposition (POD) reduced order model is applied naively (this corresponds to the naive use of (2a) in the abstract setting), then only marginal computational savings can be realized, see the row POD40 in Table 2. The DEIM reduced order model is able to deliver significant gains in computing time, see POD40/DEM40 in Table 2, while accurately representing the fingering exhibited by the subsurface flow, see Figure 6.
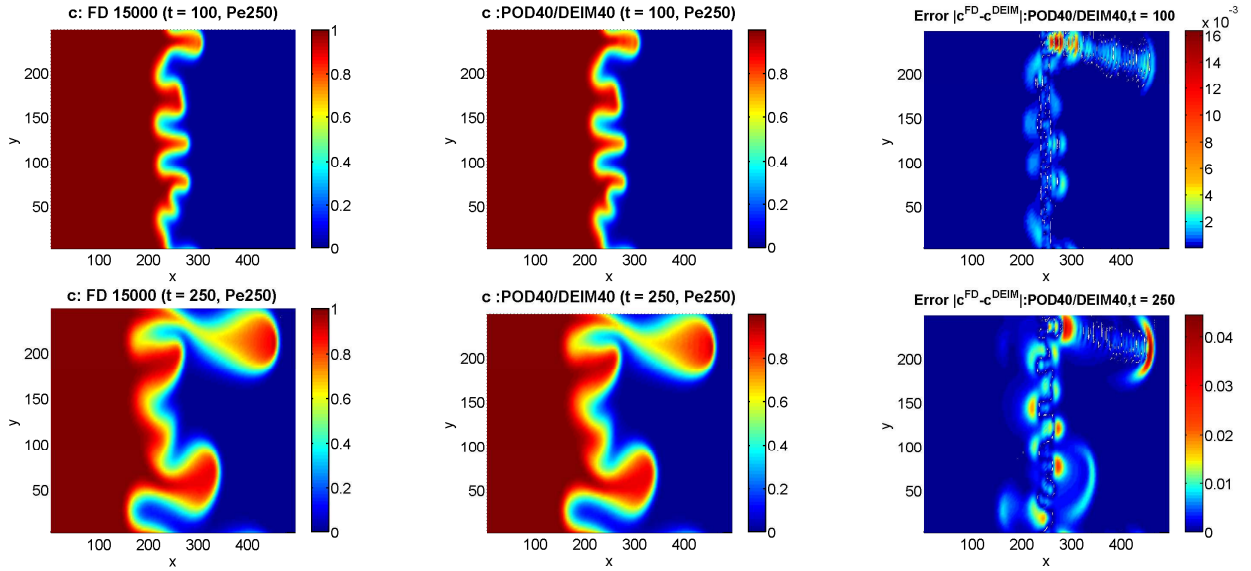

Figure 6: Concentration plots of the injected fluid (from the left half) at time t=100 and t= 250 from the full-order system of dimension 15000 and from the POD-DEIM reduced system with both POD and DEIM having dimension 40 (Peclet numbers Pe = 250).

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Dimension	Avg Rel Error of c	CPU time (sec)
Full 15000 (FD)	-	2.138×10^3
POD40	4.066×10^{-4}	2.442×10^2
POD40/DEIM40	2.045×10^{-3}	1.275

Table 2: Average relative error of the solution for the concentration and CPU time of full-order system, POD reduced system,POD-DEIM reduced system.

2.3.4 State Space Error Estimates for POD-DEIM Nonlinear Model Reduction

We have derived state space error bounds for the solutions of reduced systems constructed using POD together with the DEIM for nonlinear dynamical systems [9]. The resulting error estimates are shown to be proportional to the sums of the singular values corresponding to neglected POD basis vectors both in Galerkin projection of the reduced system and in the DEIM approximation of the nonlinear term. The analysis is particularly relevant to ODE systems arising from spatial discretizations of parabolic PDEs (e.g. convection, diffusion, reaction equations). The derivation clearly identifies where the parabolic nature of the PDE is crucial. It also explains how the DEIM approximation error involving the nonlinear term comes into play.

There are very few rigorous results concerning the accuracy of a trajectory obtained from the reduced system as an approximation to the trajectory that would have been obtained with the full system. The approach involves the application of a very nice generalization of the so called logarithimc norm to logarithmic Lipschitz constants (due to G. Soderlind). This approach applies to a fairly general class of nonlinear functions. The result gives a very convincing explanation of the observation that systems arising from spatial discretizations of parabolic PDEs often reduce dramatically. The ultimate result lends rigor to the heuristic notion that the error in trajectory approximation should be proportional to the first neglected singular value in the SVD truncation.

2.4 Model Reduction and Domain Decomposition

We have introduced a technique for the dimension reduction of a class of partial differential equation (PDE) constrained optimization problems for which the optimization variables are related to spatially localized quantities [1, 2, 3]. The semidiscrete optimization problems are of the form

$$\text{minimize} \int_0^T \ell(\mathbf{y}(t), t, \theta)dt, \tag{3a}$$

subject to

$$\mathbf{E}(\theta)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\theta)\mathbf{y}(t) = \mathbf{B}(\theta)\mathbf{u}(t), \quad t \in (0, T), \qquad \mathbf{E}(\theta)\mathbf{y}(0) = \mathbf{y}_0, \tag{3b}$$

$$\theta \in \Theta. \tag{3c}$$

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Optimal control problems and a shape optimization problems governed by advection diffusion PDEs are studied in [3]. A shape optimization problems governed by the Stokes system is investigated in [1]. The optimization parameter θ only enters the PDE in a spatially localized region if, e.g., control inputs are spatially localized or only a small portion of the domain can be modified in a shape optimization problem. This implies for the semidiscrete problem (3) that only relatively few entries of $\mathbf{E}, \mathbf{A}$, etc., depend on θ.

Our approach uses domain decomposition applied to the optimality system for (3) to isolate the subsystem that explicitly depends on the optimization variables from the remaining linear optimality subsystem. We apply balanced truncation model reduction to the linear optimality subsystem. The resulting coupled reduced optimality system can be interpreted as the optimality system of a reduced optimization problem which has the same structure as (3), but is of much smaller size.

We have derived estimates $\|\nabla J(\theta) - \nabla \widehat{J}(\theta)\| \leq c(\sigma_{n+1} + \ldots + \sigma_N)$, for all $\theta \in \Theta$, for the error in the gradient $\nabla J(\theta)$ corresponding to (3) and the gradient $\nabla \widehat{J}(\theta)$ corresponding the reduced problem in terms of the truncated Hankel singular values $\sigma_{n+1}, \ldots, \sigma_N$ of the linear optimality subsystem. This implies error estimates for the solution θ_* of (3) and the solution $\widehat{\theta}_*$ of the reduced problem $\|\theta_* - \widehat{\theta}_*\| \leq c(\sigma_{n+1} + \ldots + \sigma_N)$. Details can be found in [1,2]. Figure 7 shows results from the application of this technique to a shape optimization problem of a biochip [2].

Additionally, error bounds can also be proven with respect to some other input variables, which could make these reduced order models interesting for optimization under uncertainty in which these auxiliary inputs variables are uncertain parameters.

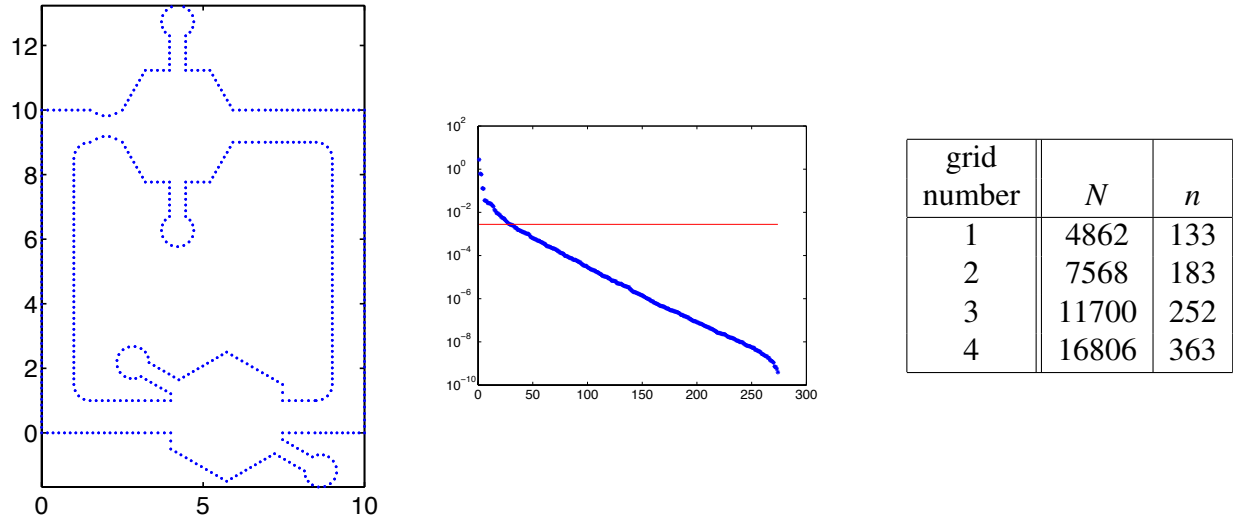| grid number	N	n
1	4862	133
2	7568	183
3	11700	252
4	16806	363

Figure 7: Left plot: The optimized shape of the biochip. Middle plot: The largest Hankel singular values and the threshold $10^{-3}\sigma_1$. Right Table: The size N of the original problem and the size n of the reduced problem for four discretizations.

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